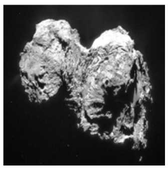
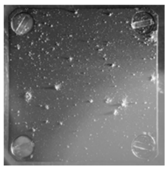


Comet 67P, ~6 km wide

Composition of cometary particles *versus* distance to sun during sample collection

- based on multivariate evaluation of mass spectral data (Rosetta/COSIMA)

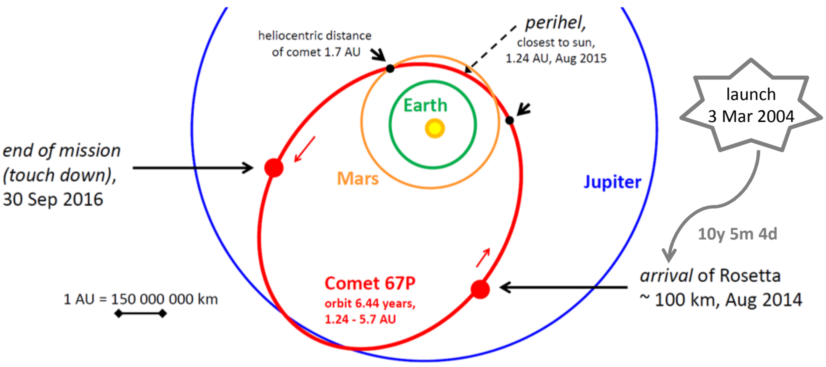


Gold target 1 cm x 1 cm with cometary particles

Varmuza Kurt [1*], Filzmoser Peter [1], Fray Nicolas [2], Cottin Hervé [2], Merouane Sihane [3], Stenzel Oliver [3], Kissel Jochen [3], Briois Christelle [4], Baklouti Donia [5], Bardyn Anais [6], Siljeström Sandra [7], Silén Johan [8], Hilchenbach Martin [3]

[1] **Vienna University of Technology**, Institute of Statistics and Mathematical Methods in Economics, Research Unit Computational Statistics, Vienna, Austria
[2] Laboratoire Interuniversitaire des Systèmes Atmosphériques, Université Paris Est Créteil et Université Paris Diderot, Créteil, France
[3] Max Planck Institute for Solar System Research, Göttingen, Germany
[4] Laboratoire de Physique et Chimie de l'Environnement et de l'Espace, Université d'Orléans et du CNES, Orléans, France
[5] Institut d'Astrophysique Spatiale, Université Paris Sud, Orsay, France
[6] DTM, Carnegie Institution of Washington, Washington, DC, USA
[7] Bioscience and Materials, Research Institute of Sweden, Stockholm, Sweden
[8] Finnish Meteorological Institute, Helsinki, Finland

Rosetta was a space mission (ESA) working more than two years (Aug 2014 to Sep 2016) near **comet** *Churyumov-Gerasimenko* (short *67P*).



COSIMA was an instrument on board of Rosetta.

It collected **cometary particles** with size 10 - 1000 µm on metal targets (distance from the comet 10 - 1500 km). More than 30,000 particles were documented by images, and more than 35,000 secondary ion mass spectra (**TOF-SIMS**) were measured on about 250 particles [1 – 7].

Particle (sample) collection occurred at heliocentric distances (from comet to sun) between 1.8 AU and 3.8 AU (AU for *Astronomical Unit*, 150 million km, approximately the mean distance between earth and sun).

Aim of this work was to check relationships between the **heliocentric distance of sampling** and **mass spectral data**.

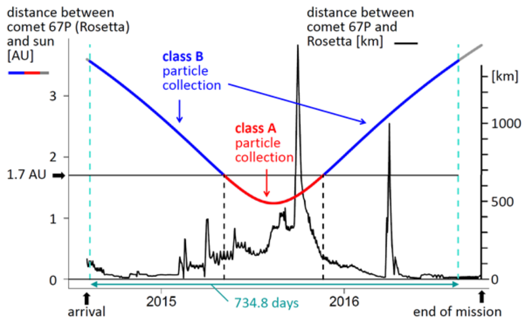
Data

n = 2863 *objects* derived from TOF-SIMS spectra measured at 256 particles, collected in 412 sampling intervals

n_1 = 1459 in **class A**: collection at ≤1.7 AU (*near* sun, warmer)

n_2 = 1404 in **class B**: collection at >1.7 AU (*far* from sun, cooler)

m = 9 variables: ion counts for C^+, CH^+, CH_2^+, CH_3^+, Mg^+, $C_2H_3^+$, $C_3H_3^+$, $C_3H_4^+$, Fe^+, normalized to sum 100 or transformed by *centered log-ratios (clr)* [compositional data].



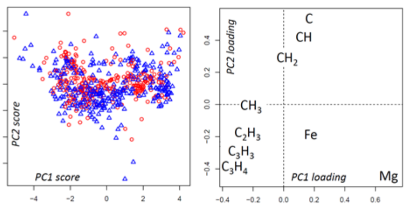
Strategy for Data Evaluation

- Characterization of the **discrimination** of **class A** (particles collected closer to sun) and **class B** (more far from sun).
- A **good discrimination indicates** a **relationship** between the used mass spectral data (characterizing the chemical composition of the particles) and the heliocentric distance of sampling.
- Methods applied: PCA; univariate distributions; KNN classification; PLS calibration; the last two with rdCV, repeated double cross validation [8].

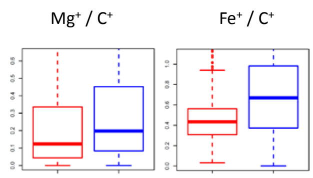
Results

PCA

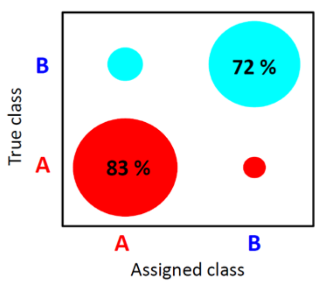
n_1 = 300
n_2 = 300
(randomly)
m = 9
clr ransf.
Variances of PC1, 2: 82.3, 10.9%

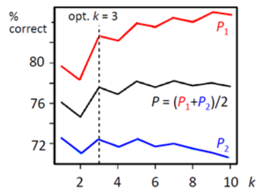


Distribution of ratios

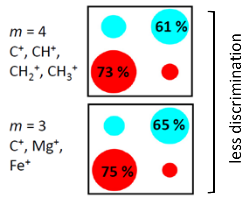


KNN classification





Repeated double cross validation: sum 100; no. segments 3 (out), 4 (in); 50 repetitions; k = 1 ... 10



PLS models (linear) *distance* = f (*spec data*) are not appropriate.

Conclusions

- The mass spectral data (characterizing the composition of the particles) are multivariate different for **class A** (collection near aphelion) and **class B** (collection more far from sun).
- KNN separates **A** and **B** well; linear approaches (PCA, PLS) do not.
- Some ion count ratios show different distributions for **A** and **B**; single ions do not.
- Influence of the **distance to the comet** or other parameters cannot be excluded.

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[2] Hilchenbach M., et al.: *The Astrophysical Journal Letters*, **816**: L32 (2016)
[3] Fray N., et al.: *Nature*, **528**, 72 (2016)
[4] Bardyn A., et al.: *MNRAS*, **469**, Suppl_2, S712 (2017)
[5] Stenzel O. et al.: *MNRAS*, **469**, Suppl_2, S492 (2017)
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* kurt.varmuza@tuwien.ac.at, http://www.lcm.tuwien.ac.at/vk/

Poster at *Conferentia Chemometrica* (CC2019), 8 - 12 Sep 2019, Karcag, Hungary

Composition of cometary particles *versus* distance to sun during sample collection - based on multivariate evaluation of mass spectral data (Rosetta/COSIMA)

Varmuza K.*[1], Filzmoser P.[1], Fray N.[2], Cottin H.[2], Merouane S.[3], Stenzel O.[3], Kissel J.[3], Briois C.[4], Baklouti D.[5], Bardyn A.[6], Siljeström S.[7], Silén J.[8], Hilchenbach M.[3]

[1] Vienna University of Technology, Institute of Statistics and Mathematical Methods in Economics, Research Unit Computational Statistics, Vienna, Austria
Email: kurt.varmuza@tuwien.ac.at
[2] Laboratoire Interuniversitaire des Systèmes Atmosphériques, Université Paris Est Créteil et Université Paris Diderot, Créteil, France
[3] Max Planck Institute for Solar System Research, Göttingen, Germany
[4] Laboratoire de Physique et Chimie de l'Environnement et de l'Espace, Université d'Orléans et du CNES, Orléans, France
[5] Institut d'Astrophysique Spatiale, Université Paris Sud, Orsay, France
[6] DTM, Carnegie Institution of Washington, Washington, DC, USA
[7] Bioscience and Materials, Research Institute of Sweden, Stockholm, Sweden
[8] Finnish Meteorological Institute, Helsinki, Finland

The instrument COSIMA [1] onboard of the ESA spacecraft Rosetta collected dust particles in the neighborhood of comet Churyumov-Gerasimenko [2]. The distance to the sun during the sample collections varied between 1.2 and 3.8 AU (AU for astronomical unit, 150 000 000 km). The chemical composition of the particle surfaces was characterized by COSIMA using TOF-SIMS (time-of-flight secondary ion mass spectrometry). A set of about 3000 spectra has been selected, and relative abundances for CH-containing positive ions (from organic compounds [3-6]) as well as elemental ions (from minerals [7]) define a set of multivariate data. Evaluation by chemometric techniques indicates different compositions of samples collected at different distances to the sun. The applied methods comprise (1) considering the compositional nature of the used mass spectral data and centered log-ratio transformation [8]; (2) robust PCA [9]; (3) KNN-classification with repeated double cross validation [10].

Supported by the Austrian Science Fund (FWF), project P 26871 - N20.

[1] Kissel J., et al.: *Space Sci. Rev.*, **128**, 823 (2007)
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Poster sessions

Monday afternoon: 15:30–16:30

Tuesday and Wendesday afternoon: 15:30–16:30

P01 Dávid Bajusz, Anita Rácz, Károly Héberger: Fingerprint similarity metrics in cheminformatics, metabolomics and other fields

P02 Barbara Biró, A. M. Sipos, A. Kovács, K. Badak-Kerti, K. Pásztor-Huszár, A. Gere: Sensory evaluation of cricket-enriched oat biscuits using check-all-that-apply analysis

P03 Zsuzsanna Guld, D. Nyitrainé Sárdy, A. Gere, A. Rácz: Multi-level comparison of Hungarian wines using advanced chemometric methods

P04 Loránd Románszki, Szilvia Klébert, and Károly Héberger: How can surface roughness be estimated at best?

P05 Sara Mostafapour, Bahram Hemmateenejad: Net analyte signal-based supervised preprocessing: application in pattern recognition

P06 Kabiruddin Ikramuddin Khan, K. Roy: Consensus QSAR modeling for the toxicity of organic chemicals against *pseudokirchneriella subcapitata* using 2D descriptors

P07 S. Lee, S. Ahn, Mihyun Kim: How to measure distribution for a pair of target classes?

P08 Péter Király, Dániel Kovács, Gergely Tóth: Remarks on some validation parameters

P09 Daniel Kovács, Péter Király, Gergely Tóth: Sample-size dependence of validation parameters

P10 Máté Mihalovits, S. Kemény: Application of regression control chart in pharmaceutical on-going stability study to detect out-of-trend results

P11 Zsolt I. Németh, I. Mészáros, Cs. Millei-Raffai, A. Vágvölgyi, R. Rákosa: Discrimination of aqueous solutions by PCA-DA assessment based on FT-IR spectrometry

P12 R. Rákosa, M. Vargovics, J. Jakab, Zsolt I. Németh: Applicability of FT-ATR-IR spectrometry in identification of *mycellium* cultures

P13 Adrián Pesti, E. Kontsek, G. Smuk, S. Gergely, A. Kiss: Mid-infrared imaging based lung cancer subtype determination

P14 Éva Pusztai, Sándor Kemény: Process capability indices when the usual assumptions fail, a tolerance interval approach

P15 Anita Rácz, Dávid Bajusz, Károly Héberger: Unsupervised data reduction: How to set the intercorrelation limits optimally.

P16 A. Rybińska-Fryca, A. Mikołajczyk, J. Łuczak, M. Paszkiewicz-Gawron, A. Zaleska-Medynska, M. Paszkiewicz and T. Puzyn: Thermal stability of ionic liquids under the conditions of synthesis of TiO2-based photocatalysts: chemometric studies

P17 Mariusz Sandomierski, Zuzanna Buchwald, Monika Zielińska, Adam Voelkel: Chemometric methods in characteristic of zeolites for specific applications

P18 L. Sipos, I. F. Boros, K. Madara, L. Csambalik, Attila Gere: Multi-criteria decision making–Comparing lettuce types by their phytonutrient content

P19 Daniel Szabó, A. Ács, F. Auer, B. Rojkovich, Gy. Nagy, P. Géher, G. Sármay, L. Drahos, K. Vékey: Analysis of protein glycosylation in *rheumatoid arthritis*

P20 Anastasia Surkova, A. Bogomolov, A. Legin, D. Kirsanov: Optical multisensor system for fat and protein determination in milk

P21 Kurt Varmuza P. Filzmoser, N. Fray, H. Cottin, S. Merouane, O. Stenzel, J. Kissel, C. Briois, D. Baklouti, A. Bardyn, S. Siljeström, J. Silén, M. Hilchenbach: Composition of cometary particles versus distance to sun during sample collection - based on multivariate evaluation of mass spectral data (Rosetta/COSIMA)

P22 Tsvetomil Voyslavov, E. Mladenova, R. Balkanska: Self-organizing maps as an approach for monofloral bee honeys botanical origin determination

P23 Máté Csontos, J. Elek, I. Bácskai, P. Arany, Infrared analysis of chemically modified 3D printed PLA scaffolds

P24 Zoran Stamenković, Ivan Pavkov, Milivoj Radojčin, Krstan Kešelj, Siniša Bikić, Attila Gere: Multicriteria optimization of raspberry convective drying processes